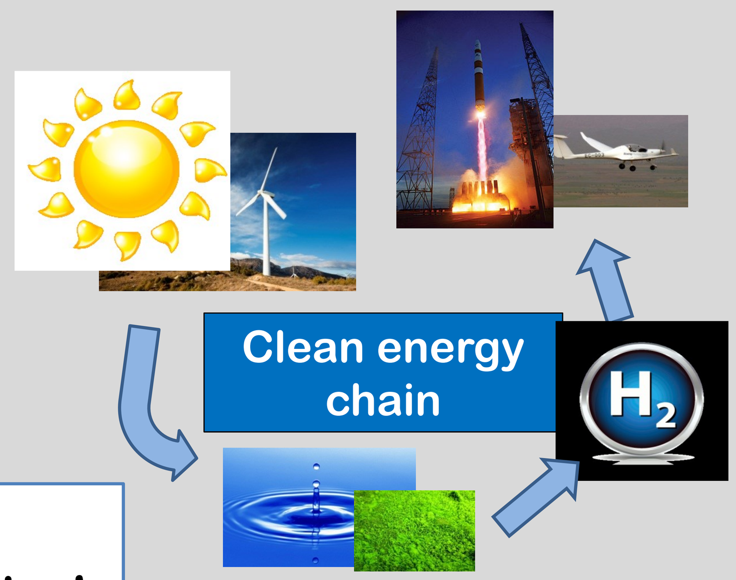
Fuel Gas Storage – The Challenge of Hydrogen

Nuno Bimbo, Jessica Sharpe, Antonio Noguera-Diaz, Andrew Physick, Leighton Holyfield, Jemma Rowlandson, Wesley Xu, Abbas Ladha, Valeska Ting and Timothy Mays.
•URL: http://people.bath.ac.uk/cestjm; : http://people.bath.ac.uk/vt233
•Department of Chemical Engineering, University of Bath, UK
•Centre for Doctoral Training in Sustainable Chemical Technologies, University of Bath, UK

Hydrogen

Global issue

- Increasing demand for energy
  - Population growth
  - Increasing wealth per capita
- Demand for new sources of energy
  - Global warming and air quality
  - Depletion of fossil fuels



Solution:
- Using hydrogen as a clean energy vector!

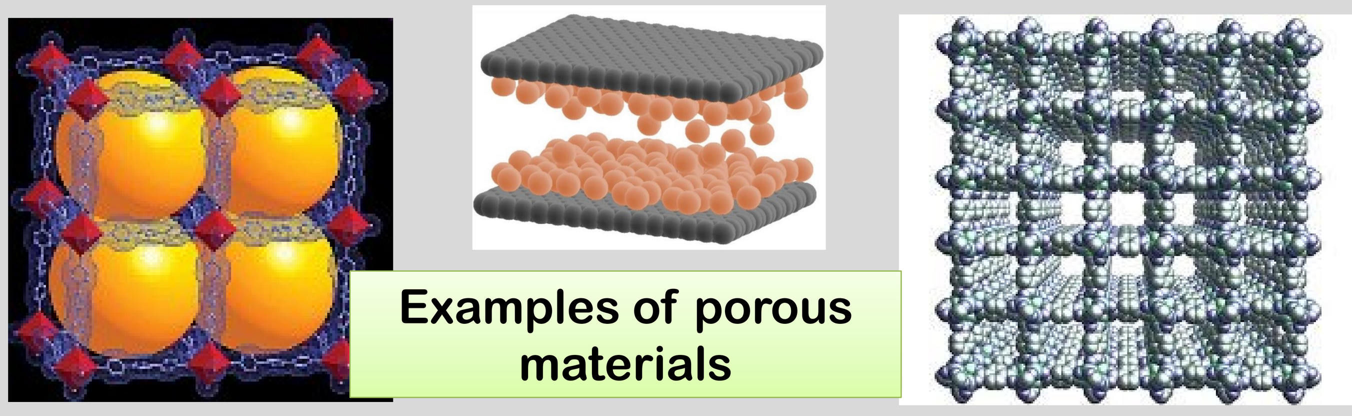
Benefits:
- Highest energy content of any chemical fuel on a mass basis
- Abundant in the form of water, biomass or hydrocarbons
- If combusted or used in a fuel cell with pure oxygen, its only product is water
- Can be used as a wide-scale clean energy vector

Hydrogen storage

Problem:
- Hydrogen has a very low density
- Conventional methods of increasing the density is to compress or liquefy
- BUT, these require unfavourable conditions.

Examples of compression and liquefaction H_2 tanks

Solution:
- Adsorb the hydrogen inside nanoporous materials!



Examples of porous materials

Hydrogen Storage in Porous Materials

Materials

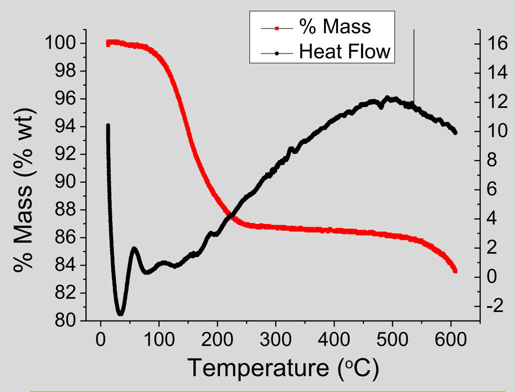
We synthesise, characterise, analyse and model a variety of different types of nanoporous materials including:

- Metal-organic frameworks
- Polymers of intrinsic microporosity
- Activated carbons
- Zeolites

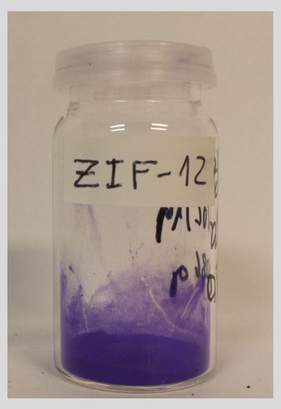
Example synthesis: ZIF-12

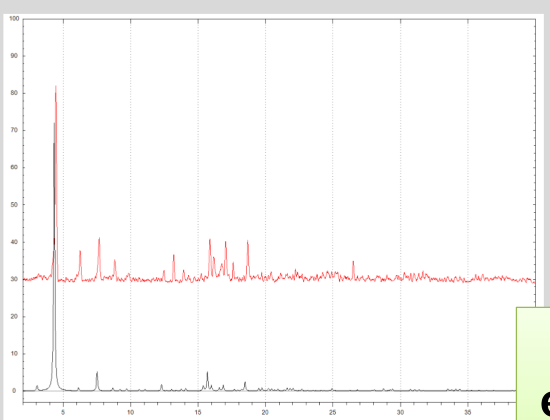
Synthetic route:

$$(CH_3COO)_2Co \cdot 4H_2O + BIM \xrightarrow[\text{RT, 3 hrs}]{\text{Methanol, Toluene, Ammonia}} Co(PhIM)_2$$



ZIF-12 TGA



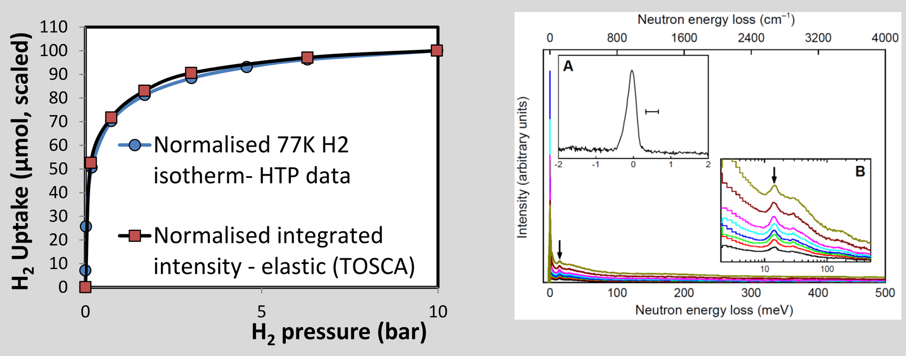


ZIF-12 XRD. Red: experimental data; Black: from CIF file

Analysis

Inelastic neutron scattering

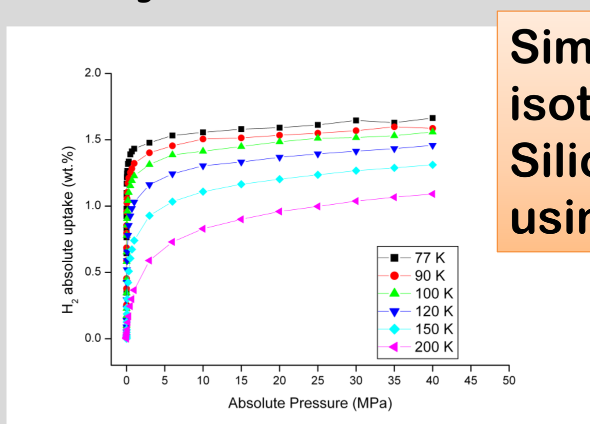
We used inelastic neutron scattering as it allowed for the verification of our model



INS integrated elastic peak and spectra for TE7

Computer simulations

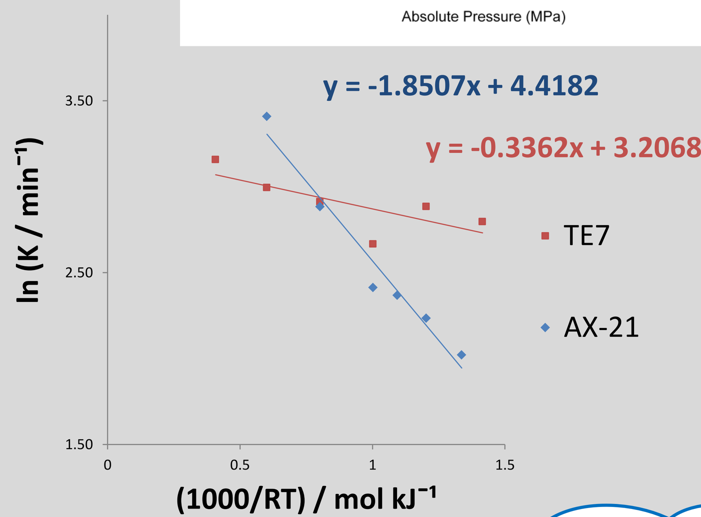
We use computer simulations in order to verify our model, and to study the molecular dynamics of the system



Simulated isotherms for Silicalite-1 using MUSIC

Kinetics

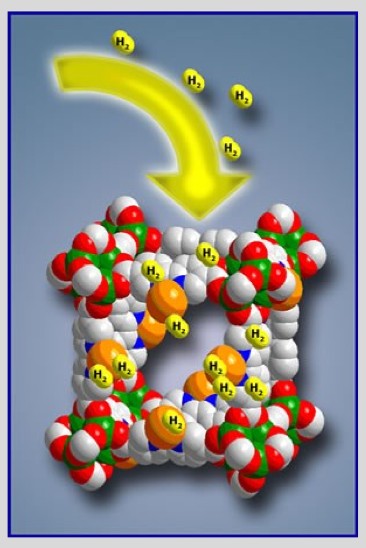
We have studied the kinetics of hydrogen adsorption for some carbons and shown that the mass transfer coefficients follow an Arrhenius relationship



Arrhenius plot of mass transfer coefficients as a function of temperature

Analysis

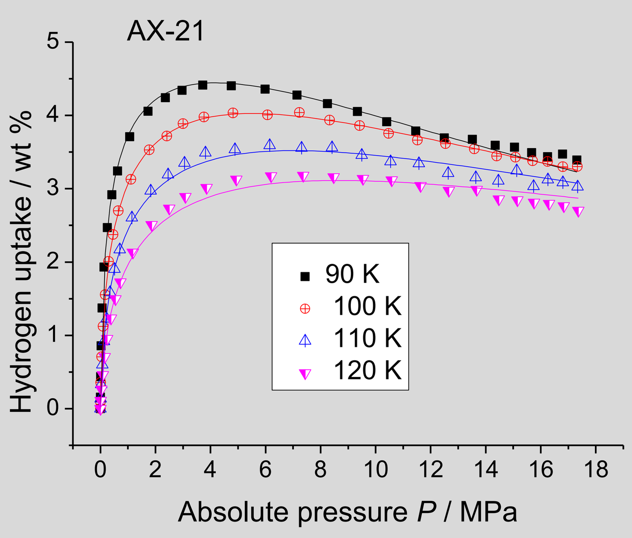
We do the analysis and modelling of excess isotherms, in order to compare with alternative storage methods, and to study the fundamentals of the adsorption process.



$$m_E = (\rho_A - \rho_B) V_P \theta_A$$

m_E = excess uptake
ρ_A = adsorbate density
ρ_B = bulk density
V_P = pore volume
Θ_A = fill factor

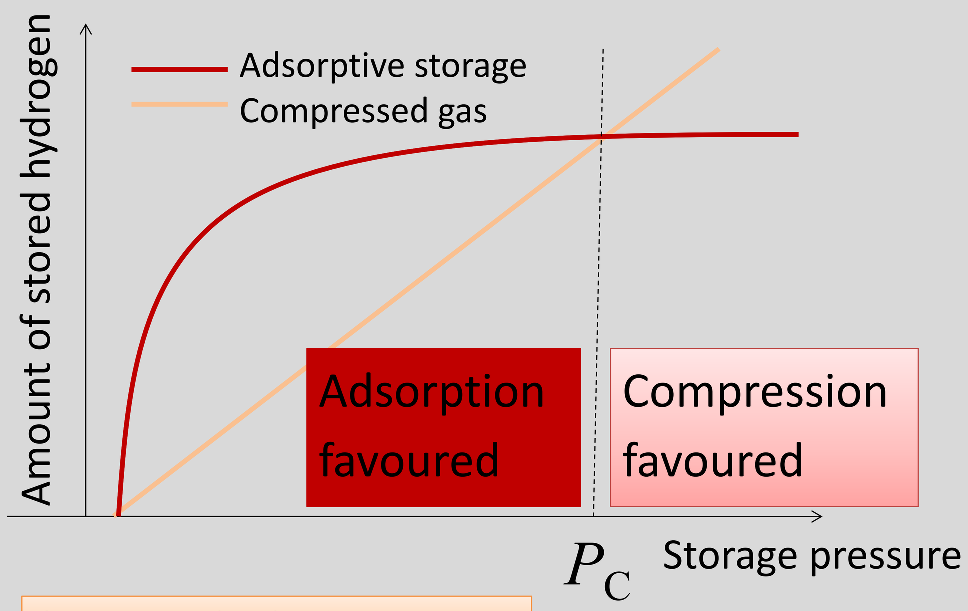
The analysis allows us to determine the optimum conditions for physisorption



Experimental high-pressure hydrogen excess and fitted isotherms for AX-21

Systems

- The analysis has been expanded to calculate the amount of hydrogen stored in tanks containing varying quantities of adsorbent, at any pressure or temperature.
- From these calculations we are able to produce design curves, which compare the amount of hydrogen stored via adsorption *vs.* the amount stored via compression at the same conditions.
- We found that there is a critical pressure, above which compression always stores more hydrogen than adsorption.



An example design curve

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